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**PROGRAM BREMS: A CODE DESIGNED TO CREATE A
BREMSSTRAHLUNG DATA BASE IN THE ENDL FORMAT**

by

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PROGRAM BREMS: A CODE DESIGNED TO CREATE A BREMSSTRAHLUNG DATA BASE IN THE ENDL FORMAT

INTRODUCTION

The computer code BREMS starts from the latest bremsstrahlung data of S. M. Seltzer and M. J. Berger (NBS) which is given in tabular form over the electron energy range 1 KeV to 10 GeV for elements with Z = 1 to 100. This data is extended to the energy range 10 eV to 100 GeV and converted to an accurately interpolable form in the ENDL format, which can be more easily used in applications.

CODE DOCUMENTATION

This code is one of a series of codes which are used to create a set of coupled electron-photon data bases which can be used in a wide variety of applications.

These codes are designed to be self documenting, in the sense that the latest documentation for each code is included as comment lines at the beginning of each code. Printed documentation, such as this document, are periodically published and consists mostly of a copy of the comment lines from the beginning of each code. The user should be aware that the comment lines within the codes are continually updated to reflect the most recent status of the codes and these comments should always be considered to be the most recent documentation for the codes and may supercede published documentation, such as this document. Therefore the user is advised to always read the documentation within the actual code which is being used.

The remainder of this report consists of a listing of the documentation which appears at the beginning of program BREMS and example output in graphic form to illustrate the systematics (i.e., versus Z) of the results. See also, "The Livermore Bremsstrahlung Data Base," UCID-21627 by D. E. Cullen and S. T. Perkins, (1989), Lawrence Livermore National National Laboratory, Livermore, CA for a discussion of the methods used by the computer code.

PROGRAM BREMS

VERSION 89-1 (JANUARY 1989)

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PURPOSE

This program converts the Seltzer and Berger bremsstrahlung data (Ref. 1 and 2) to the ENDL format (Ref. 3) in an accurate form suitable for use in applications. In addition output may be obtained in the PLOTTAB format suitable for plotting.

METHOD

The Seltzer and Berger data is presented in tabulated form for all elements between Z = 1 and 100. For each element data is given at 31 incident electron energies between 1 keV and 10 GeV. At each incident energy the photon spectrum is defined at 14 ratios of the photon energy to the incident electron energy where the ratio varies between 0 and 1. Seltzer and Berger do not state how to interpolate between their tabulated values. For use in applications we require data for incident electron energies between 10 eV and 100 GeV and we must be able to accurately interpolate to define the spectrum at all incident electron energies and all photon energies. In order to meet this need this program performs cubic spline fits to the data, in order to define the data at all energies, and uses the systematics of the data to extend it down to 10 eV and up to 100 GeV. After fitting and extending the data in energy the data is reduced to a table that can be accurately interpolated using any combination of linear or log variation in energy and spectra that the user of this code specifies by input.

RESULTS

This program can calculate

- (1) Cross section**
- (2) Photon spectra**
- (3) Spectrum averaged photon energy**
- (4) Spectrum averaged secondary electron energy**
- (5) Average photon energy times cross section**
- (6) The extended Seltzer and Berger data**
- (7) Seltzer and Berger's phirad parameter (see: Ref. 1 and 2)**

Items (1)-(4) can be optionally output in the ENDL format.

Items (1)-(7) can be optionally output in the PLOTTAB format.

ACCURACY OF THE RESULTS

All results will be produced in the form of tables. For use in applications it is important that the results be known not only at the tabulated values, but rather at all values. In order to allow this the program will produce a sufficient number of data points to allow accurate interpolation between tabulated points. By input the user may specify how to interpolate in incident electron energy vs. cross section or average energy (electron and photon) and photon energy vs. spectrum (at each incident electron energy). Any combination of linear and/or log interpolation may be specified. It should be mentioned that in terms of size of the output files created by this program the spectra file is by far the largest. Since over a large portion of the photon energy range the spectra vary as $1/E$, the spectra can be accurately represented in a very compact form if one uses log-log interpolation in photon energy vs. spectra.

METHOD

The user specifies by input the Z range (elements) of the data to be translated. Next the user specifies what interpolation laws to use. Finally the user specifies the output format of the data. For each requested Z the program will first perform a cubic spline fit to each of the 14 photon/electron energy curves to define the spectrum vs. incident electron energy. The local value, slope and curvature near 1 keV is then used to extend the data down to 10 eV. Next the local value and slope near 10 GeV is used to extend the data up to 100 GeV along a saturation curve - $\gamma + \beta(1 - \exp(\alpha(T-K)))$ where,

T = incident electron energy

K = photon energy

Gamma = value for T = W

Alpha = defined to match value and slope of each curve

Beta = defined to match value and slope of each curve

The cubic spline parameters and extension of the data in energy is next used to define the minimum number of incident energy points required to allow accurate interpolation along all of the 14 curves (in order to define a uniform incident energy grid). Next, at each incident energy a cubic spline fit is performed to the spectrum vs. photon energy. The cubic spline parameters are then used to define the minimum number of photon energy points to allow accurate interpolation of the spectrum. The data is then output in the format(s) selected by the user.

INPUT PARAMETERS

Three lines of input are required for each calculation. The three lines may be repeated any number of times. Requested Z ranges must be in ascending, non-overlapping Z order. Each input field occupies 11 columns and data may be entered anywhere within these 11 columns (e.g., integers need not be right adjusted). All input will be read as characters and then converted internally. If any input field is zero (or blank) the appropriate variable will be set equal to the default value defined below.

Line	Columns	Format	Default	Definition
1	1-11 12-22 23-33	I11 I11 I11	1 100 0	Minimum Z Maximum Z Date (yyymmdd) for ENDL output
2	1-11 12-22 23-33 34-44	I11 D11.4 I11 D11.4	2 0.01 2 0.01	Cross section interpolation law Cross section interpolation uncertainty (i.e., 1 per-cent) Spectra interpolation law Spectra interpolation uncertainty (i.e., 1 per-cent)
				Note, the cross section and average energies all use the same interpolation law.
				Note, the interpolation law is defined to be, = 2 lin E vs. lin spectrum (cross section) = 3 lin E vs. log spectrum (cross section) = 4 log E vs. lin spectrum (cross section) = 5 log E vs. log spectrum (cross section)
3	1-11 12-22 23-33 34-44 45-55 56-66	I11 I11 I11 I11 I11 I11	0 0 0 0 0 0	Cross section output format Spectra output format Photon energy * cross section Extended Seltzer and Berger data Phirad Output report = 0 - on line = 1 - to file
				Note, when cross section output is requested cross sections and average energies will also be output.
				Note, only cross sections, spectra and average energy can be output in the ENDL format, but any of these parameters may be output in the PLOTTAB format.
				Note, the available output formats are, = 0 none = 1 ENDL = 2 PLOTTAB = 3 ENDL and PLOTTAB

EXAMPLE INPUT

Translate the silver ($Z=47$) data and use a date of 890215 for any ENDL formatted output. Cross section and spectra should be log – log interpolatable to within 1 per-cent (0.01 as a fraction). Output cross sections and spectra in the ENDL format. The following 3 lines are required as input,

47	47	890215		
5	0.01	5	0.01	
1	1	0	0	0

These three lines may be followed by additional sets of 3 lines specifying the next calculation. Calculations will continue until all set of input requests have been processed (i.e., until an end of file is read on the input parameter file).

I/O FILE DEFINITIONS

Unit	Filename	Definition
5	INBREMS	Input parameters
6	REPORT	Output report
10	BREMSIN	Seltzer and Berger data
11	PLOTTAB	PLOTTAB formatted output
12	SPECTRA	Photon spectra (ENDL format)
14	CROSS	Cross sections (ENDL format)
15	PHOTON	Average photon energy (ENDL format)
16	ELECTRON	Average electron secondary energy (ENDL)
17	STPIN	Atomic weights (for ENDL format)

REFERENCES

1. S. M. Seltzer and M. J. Berger, "Bremsstrahlung Spectra From Electron Interactions With Screened Atomic Nuclei and Orbital Electrons," Nuclear Instruments and Methods in Physics Research B12, 95–134 (1985).
2. S. M. Seltzer and M. J. Berger, "Bremsstrahlung Energy Spectra From Electrons With Kinetic Energy 1 keV to 10 GeV Incident on Screened Nuclei and Orbital Electrons of Neutral Atoms With $Z = 1\text{--}100$, Atomic Data and Nuclear Data Tables," Vol. 35, No. 3 (1986).
3. R. J. Howerton, et al, "Omega: A Cray 1 Executive Code For the LLNL Nuclear Data Libraries," Lawrence Livermore National Laboratory, Livermore, CA, UCRL-50400, Vol. 25, (1983).

COMPUTER DEPENDENT CODING

The computer dependent coding in this program includes,

(1) CHARACTER/INTEGER

Treat character arrays either as character (Fortran-77 convention) or integer (Fortran-H convention).

(2) DOUBLE/SINGLE

Treat energy dependent variables in single or double precision. On long word length computers (e.g., Cray) this program can be optimized by using single precision. On short word length computers (e.g., IBM) double precision must be used.

(3) NAMES

Option to use standard file names

(4) CIVIC

Livermore CIVIC compiler conventions

(5) STOP/EXIT

The program can terminate execution using either call exit or stop

Program CONVERT may be used to automatically convert this program back and forth using any combination of these computer dependent options to best meet your needs (for details of program CONVERT contact D. E. Cullen at the above address).

EXAMPLE: INPUT PARAMETERS AND OUTPUT REPORT

The following 3 lines of input parameters will produce the following output report.

```
1      30    890215
5      0.001      5      0.01
2          0      0          0      0      1
```

CREATE A BREMSSTRAHLUNG DATA BASE IN THE ENDL FORMAT (BREMS 89-1)

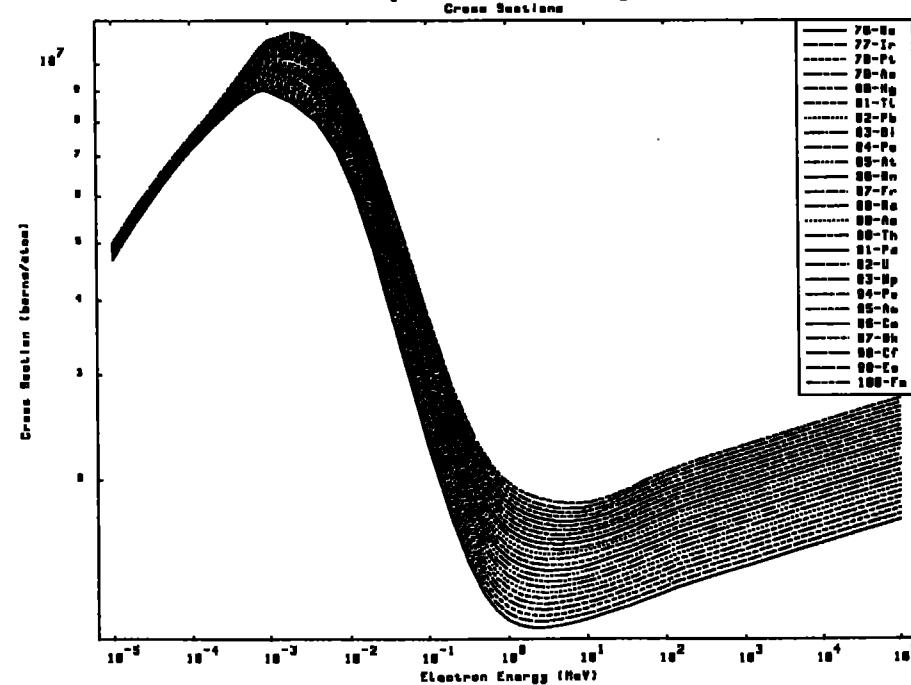
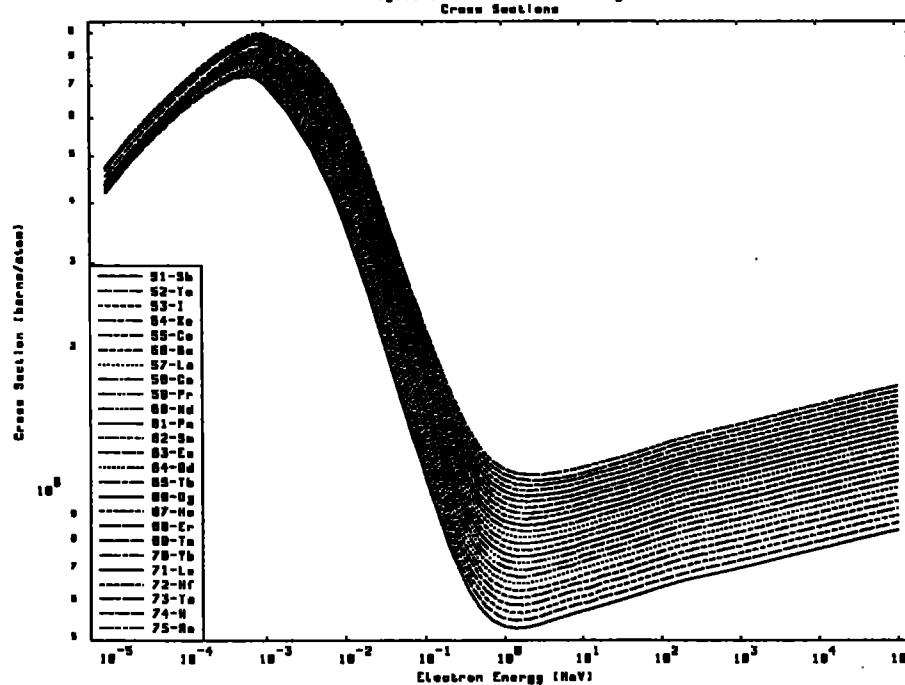
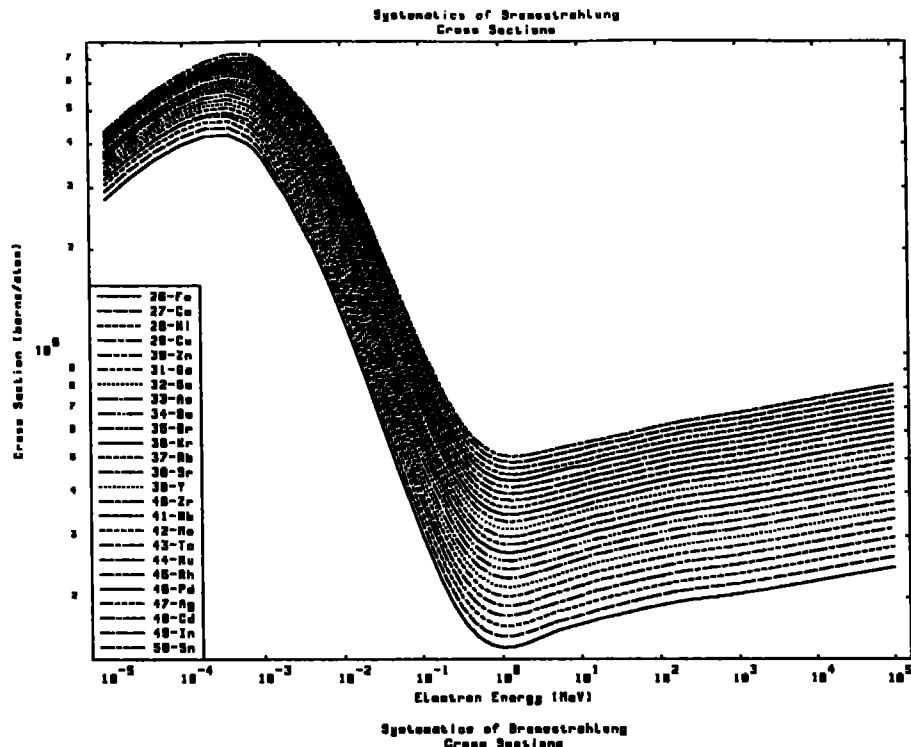
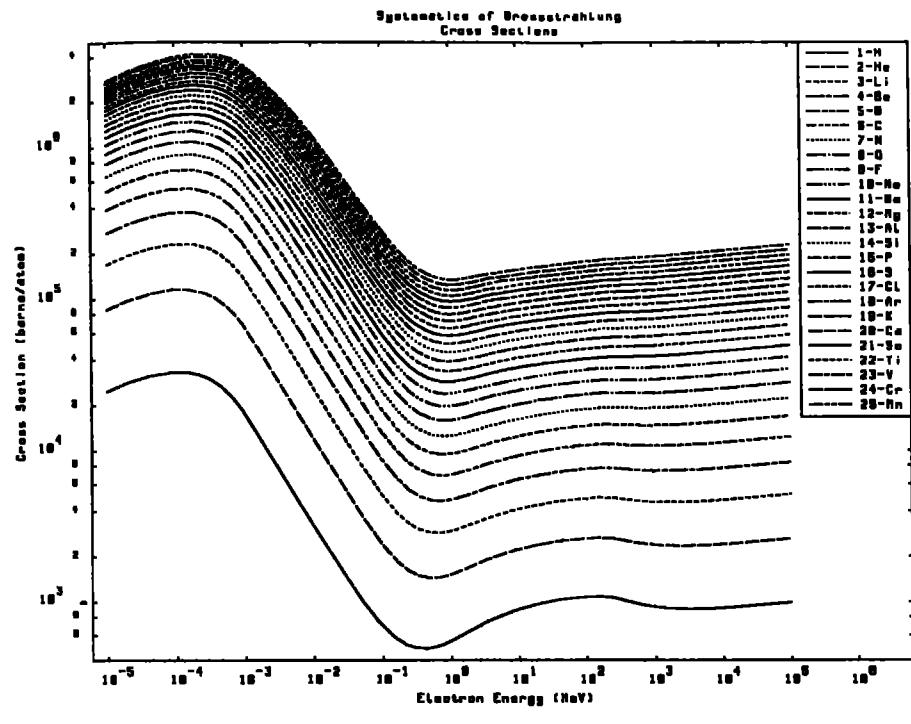
INTERPRETATION OF INPUT PARAMETERS

Z RANGE.....	1 TO	30
DATE.....	890215	
CROSS SECTION.....	LOG E VS. LOG Y	1.00000- 3 (0.1000 %)
SPECTRA.....	LOG E VS. LOG Y	1.00000- 2 (1.0000 %)
CROSS SECTION OUTPUT.....	PLOTTAB	
SPECTRA OUTPUT.....	NONE	
ENERGY * CROSS SECTION.....	NONE	
EXTENDED SELTZER AND BERGER DATA..	NONE	
PHIRAD.....	NONE	
OUTPUT.....	TO FILE	

ELEMENT	ATOMIC WEIGHT	CROSS SECTION POINTS	SPECTRA POINTS
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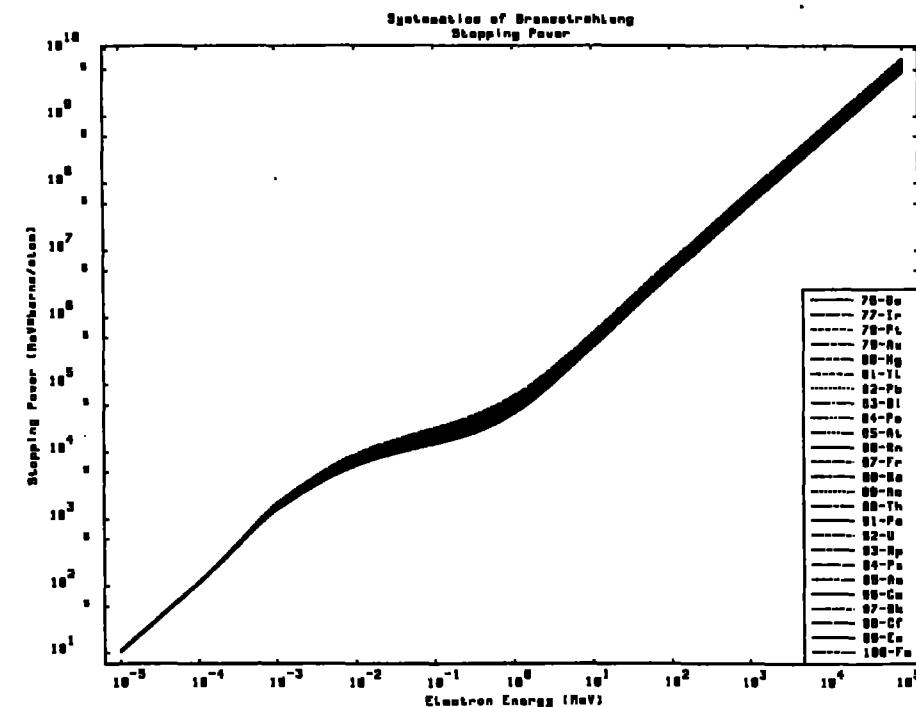
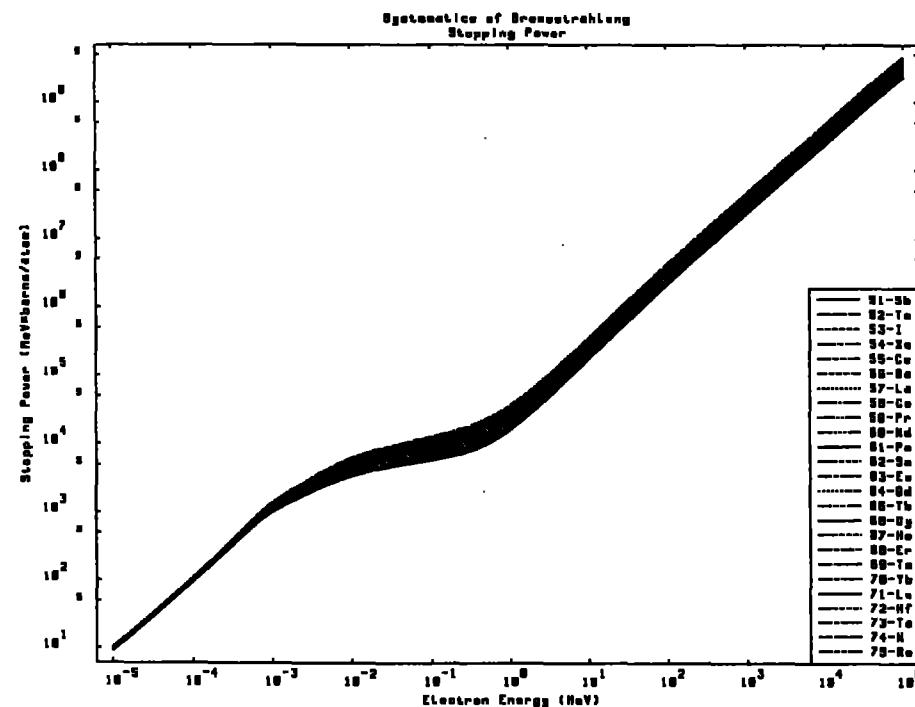
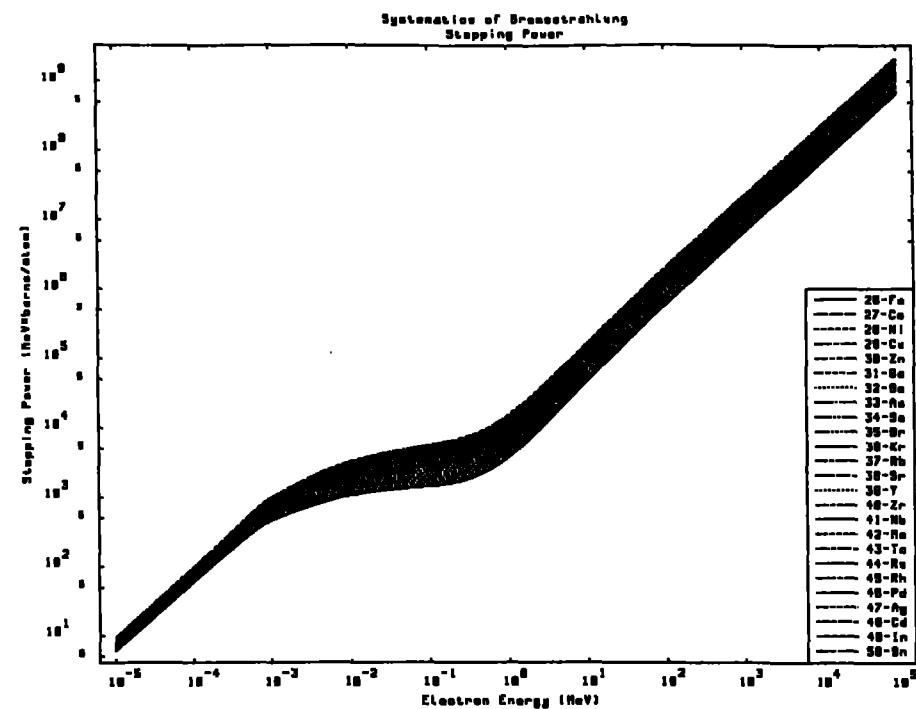
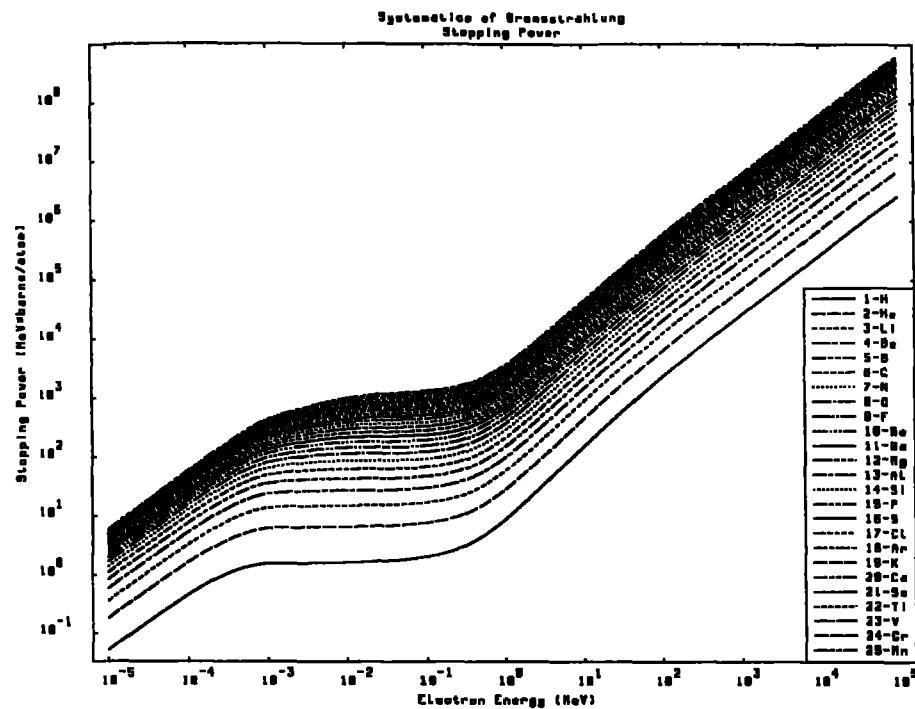
1-H	1.0080	47	982
2-He	4.0026	43	839
3-Li	6.9390	42	800
4-Be	9.0122	42	777
5-B	10.8110	42	758
6-C	12.0112	41	722
7-N	14.0067	41	712
8-O	15.9994	42	723
9-F	18.9984	41	699
10-Ne	20.1790	42	718
11-Na	22.9898	41	691
12-Mg	24.3120	42	707
13-Al	26.9815	43	727
14-Si	28.0860	42	709
15-P	30.9738	42	690
16-S	32.0640	43	719
17-Cl	35.4530	43	719
18-Ar	39.9480	43	720
19-K	39.1020	43	717
20-Ca	40.0800	43	708
21-Sc	44.9580	44	743
22-Ti	47.9000	43	715
23-V	50.9420	43	709
24-Cr	51.9960	43	713
25-Mn	54.9380	43	711
26-Fe	55.8470	43	710
27-Co	58.9332	43	702
28-Ni	58.7100	43	702
29-Cu	63.5400	43	703
30-Zn	65.3700	43	711

Example Results:
Systematics of Bremsstrahlung Cross Sections

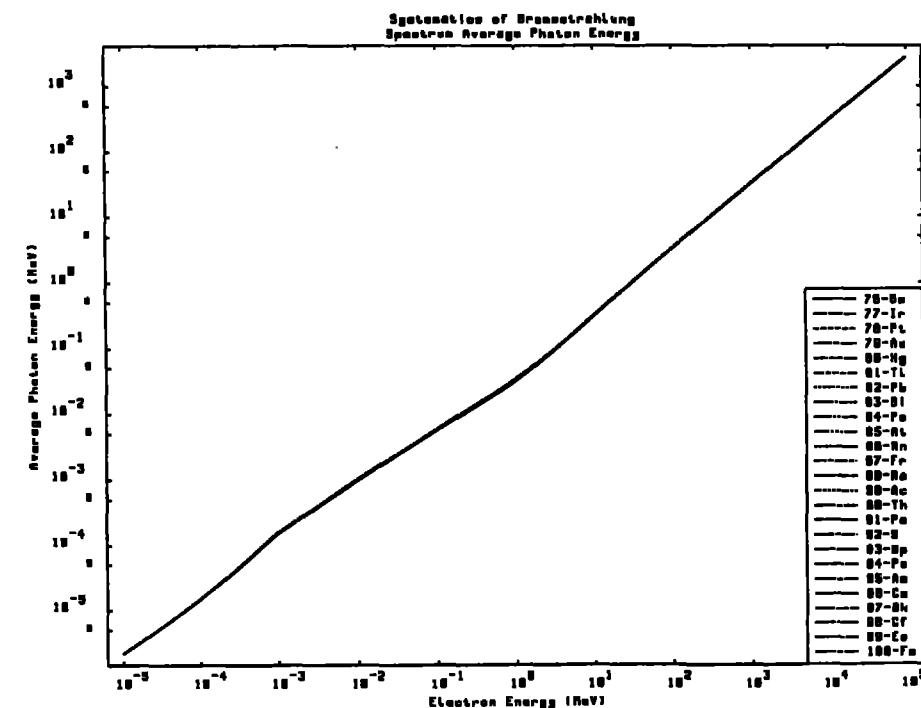
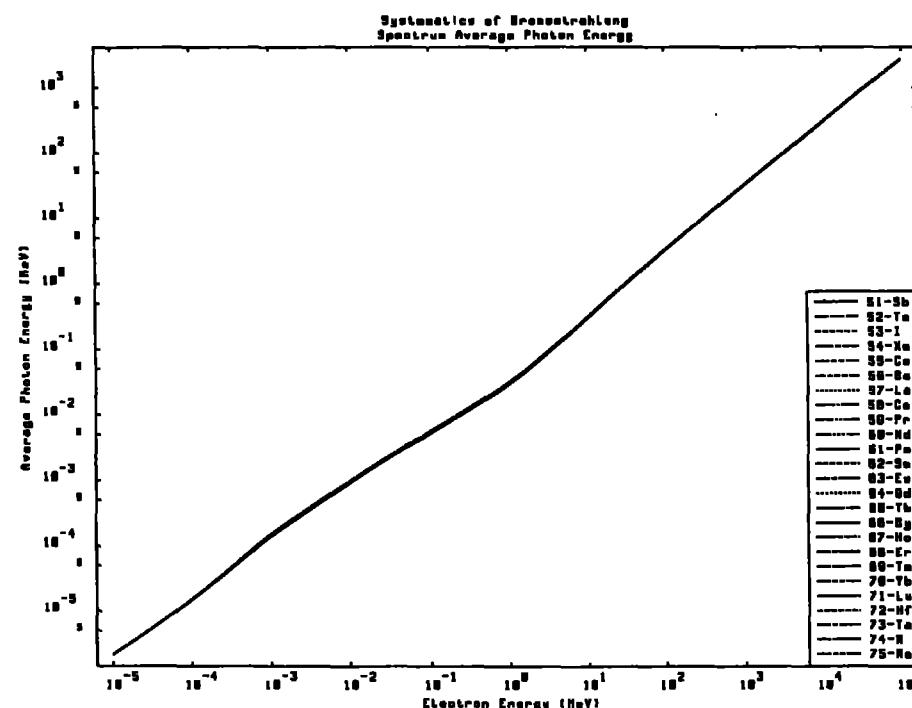
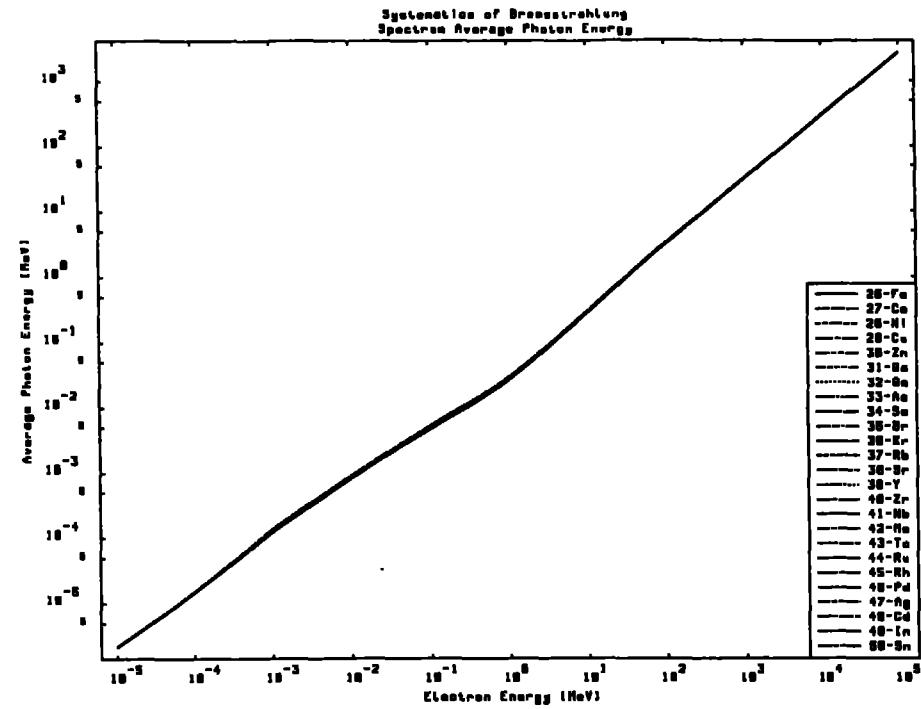
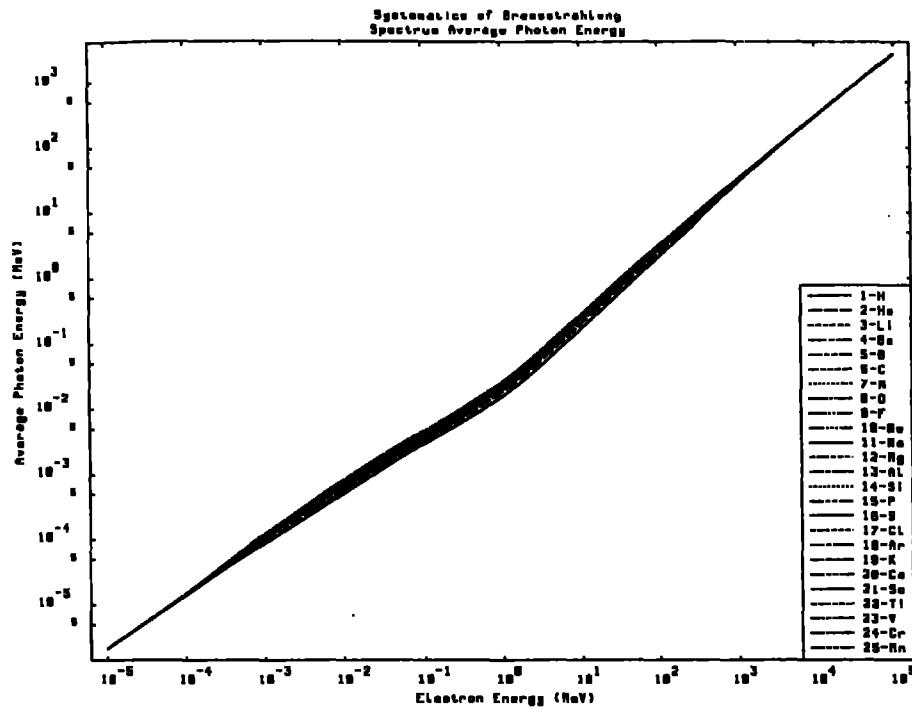


Example Results:
Systematics of Bremsstrahlung Stopping Power

Note, stopping power is proportional to the integral of the bremsstrahlung photon spectrum multiplied by the photon energy integrated over all photon energies. It is this quantity which is presented on the following page and identified as stopping power. This quantity may be thought of as the stopping power per atom; in order to define the actual stopping power one would have to include the effect of atom density.



Example Results:
Systematics of bremsstrahlung
spectrum average photon energy

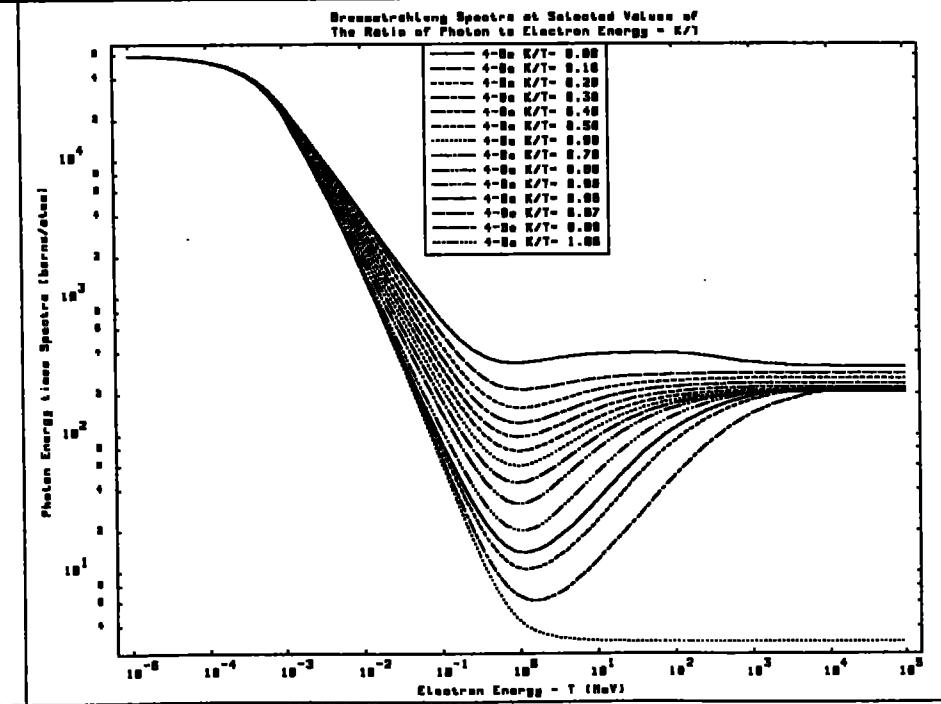
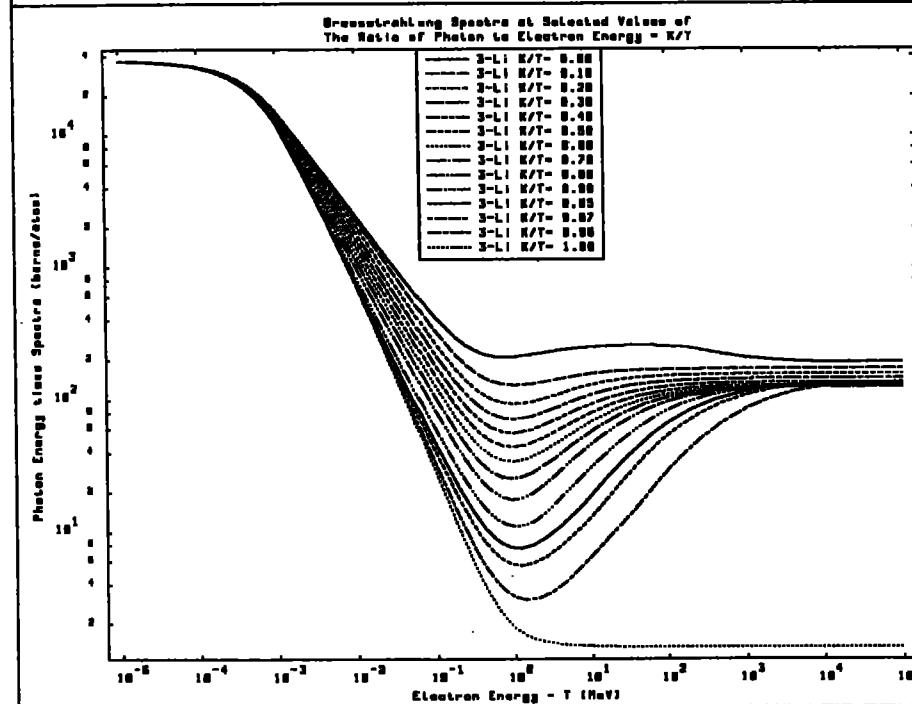
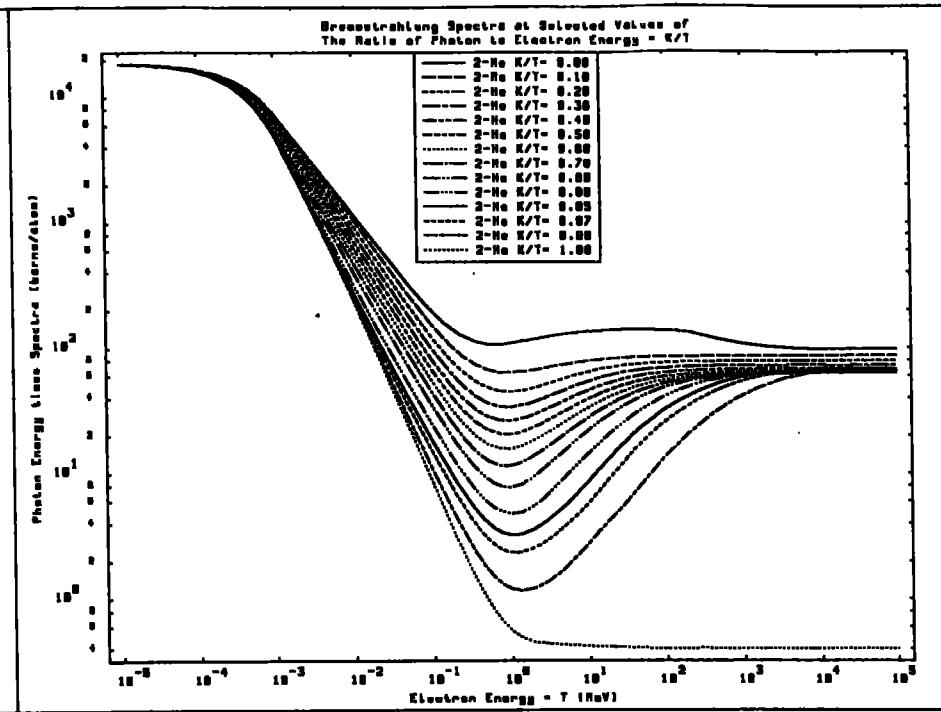
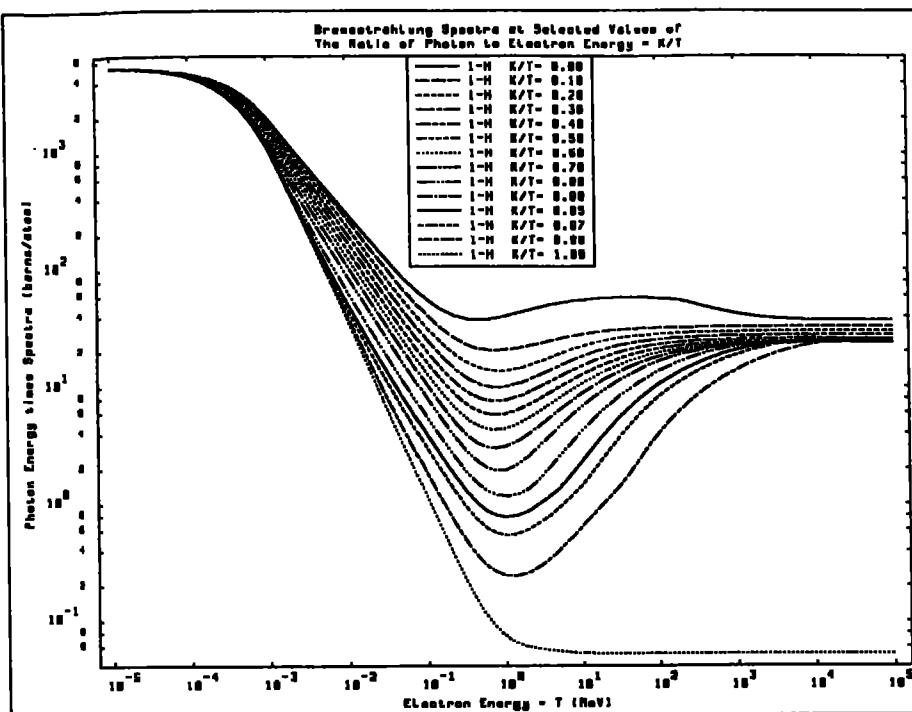


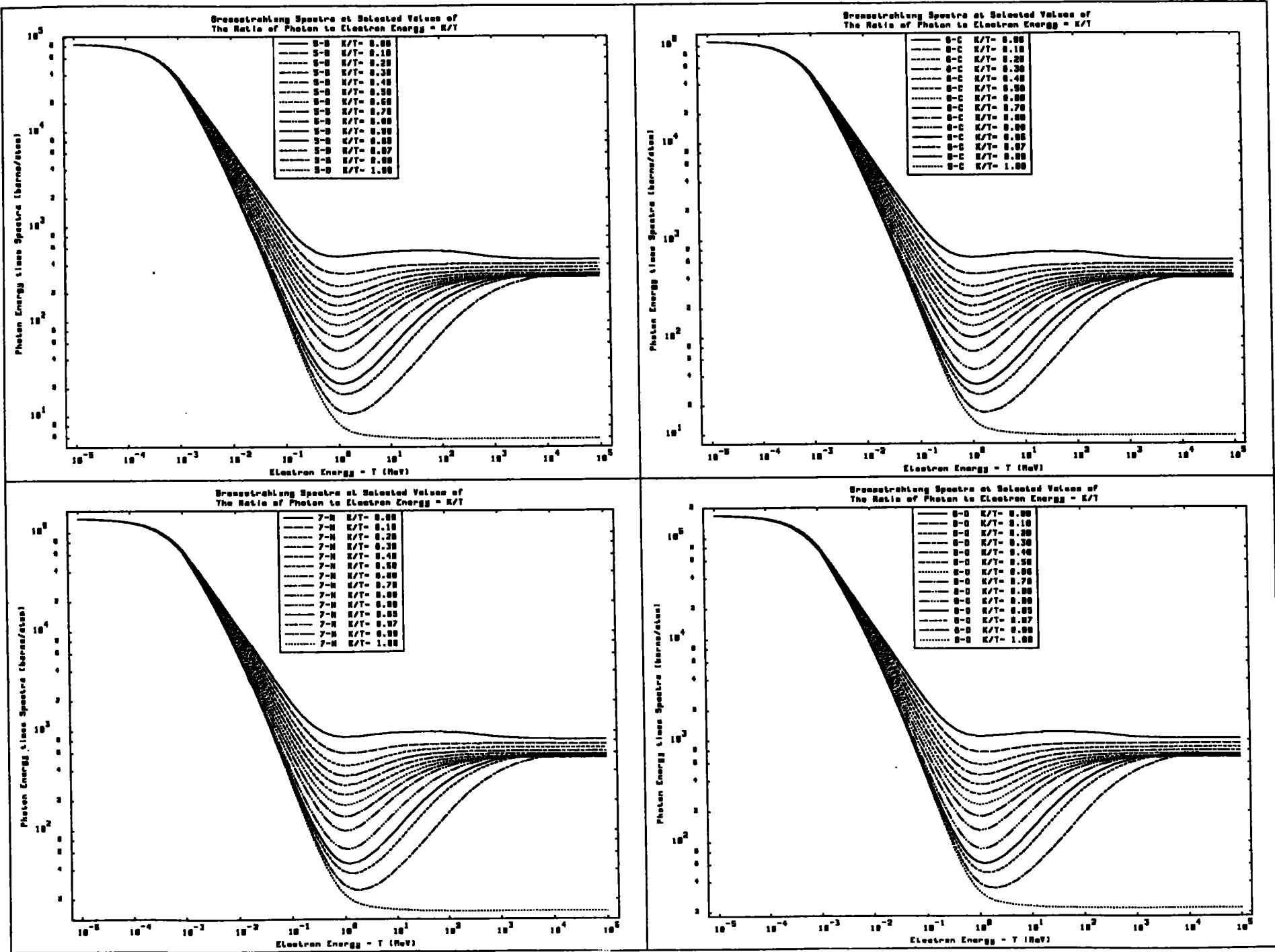
Example Results:

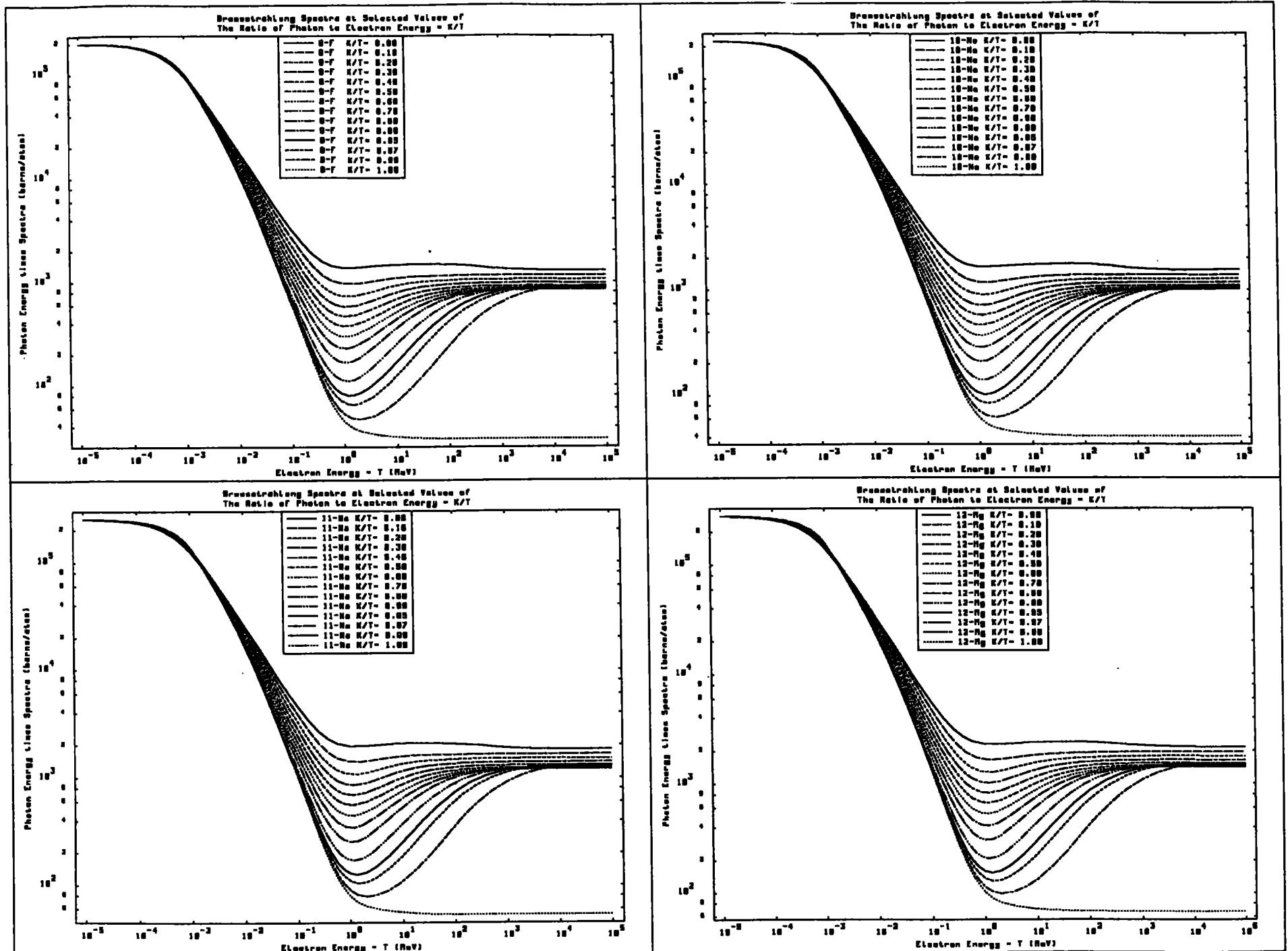
**Bremsstrahlung Spectra at Selected Values of
The Ratio of Photon to Electron Energy = K/T**

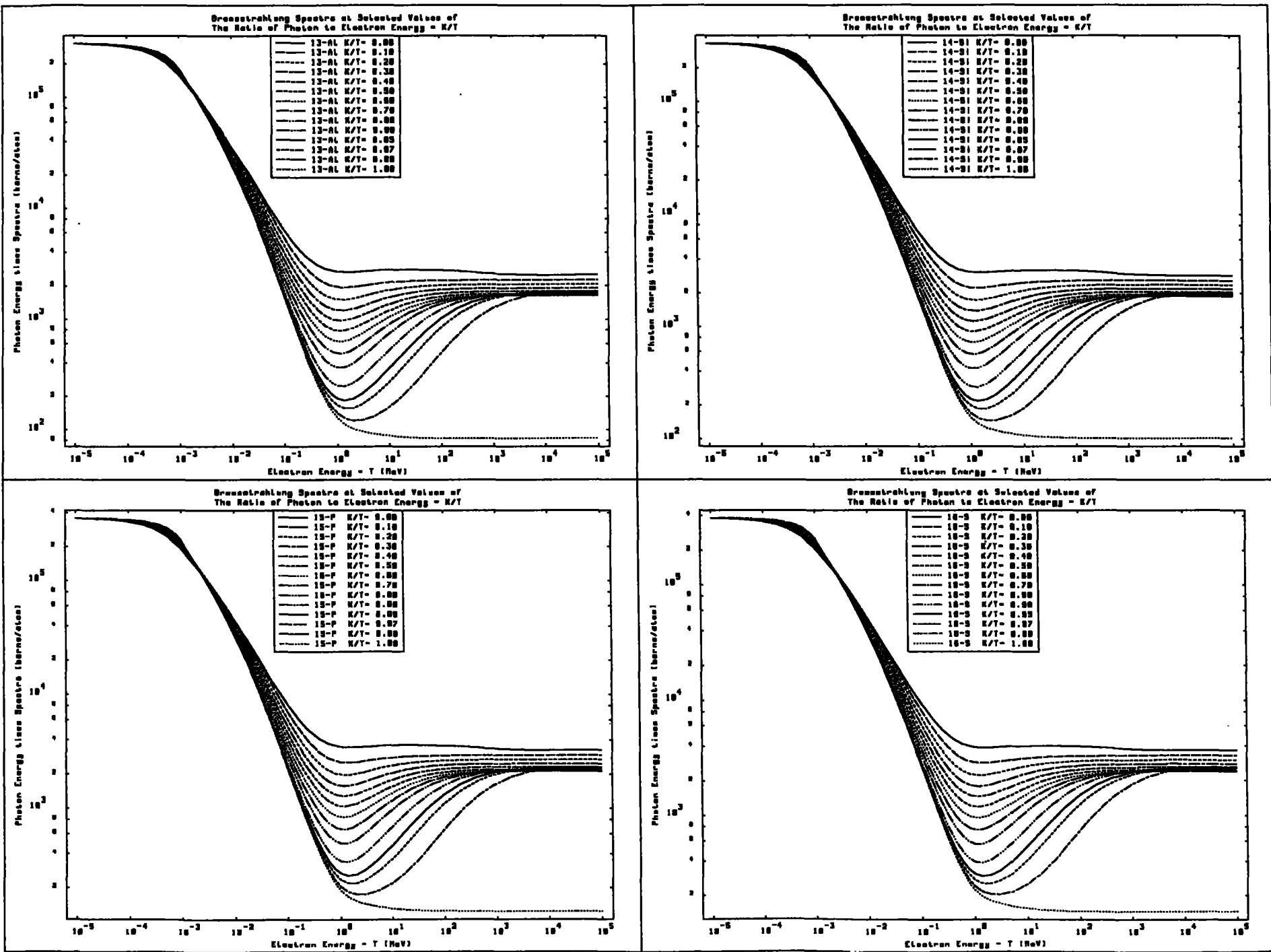
On the following pages for each element $Z = 1$ to 100 photon energy times the spectra is presented for 14 ratios of the photon energy (K) to the electron energy (T). From these figures for any given element and any given electron energy it may be seen how the energy is distributed among the emitted photons.

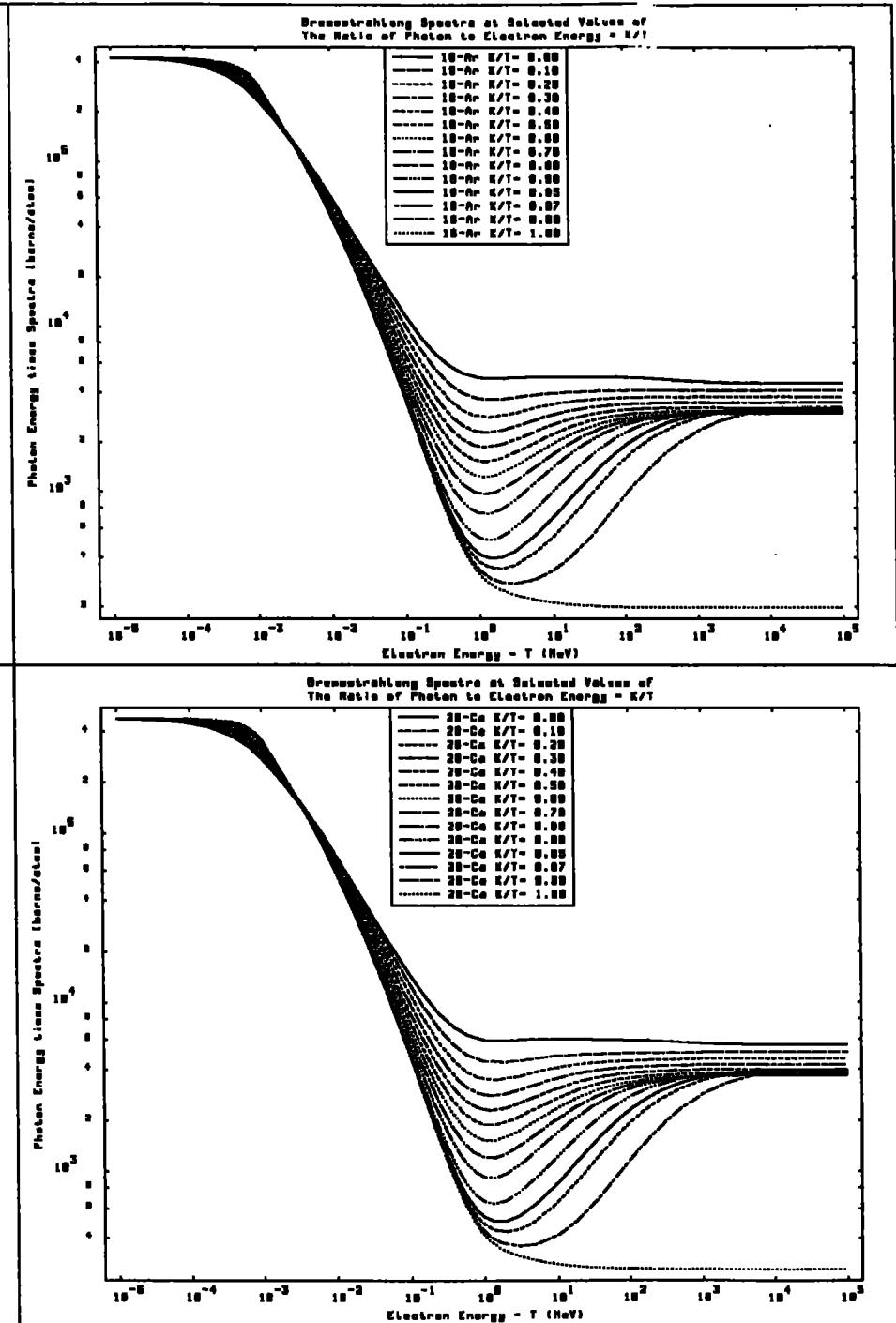
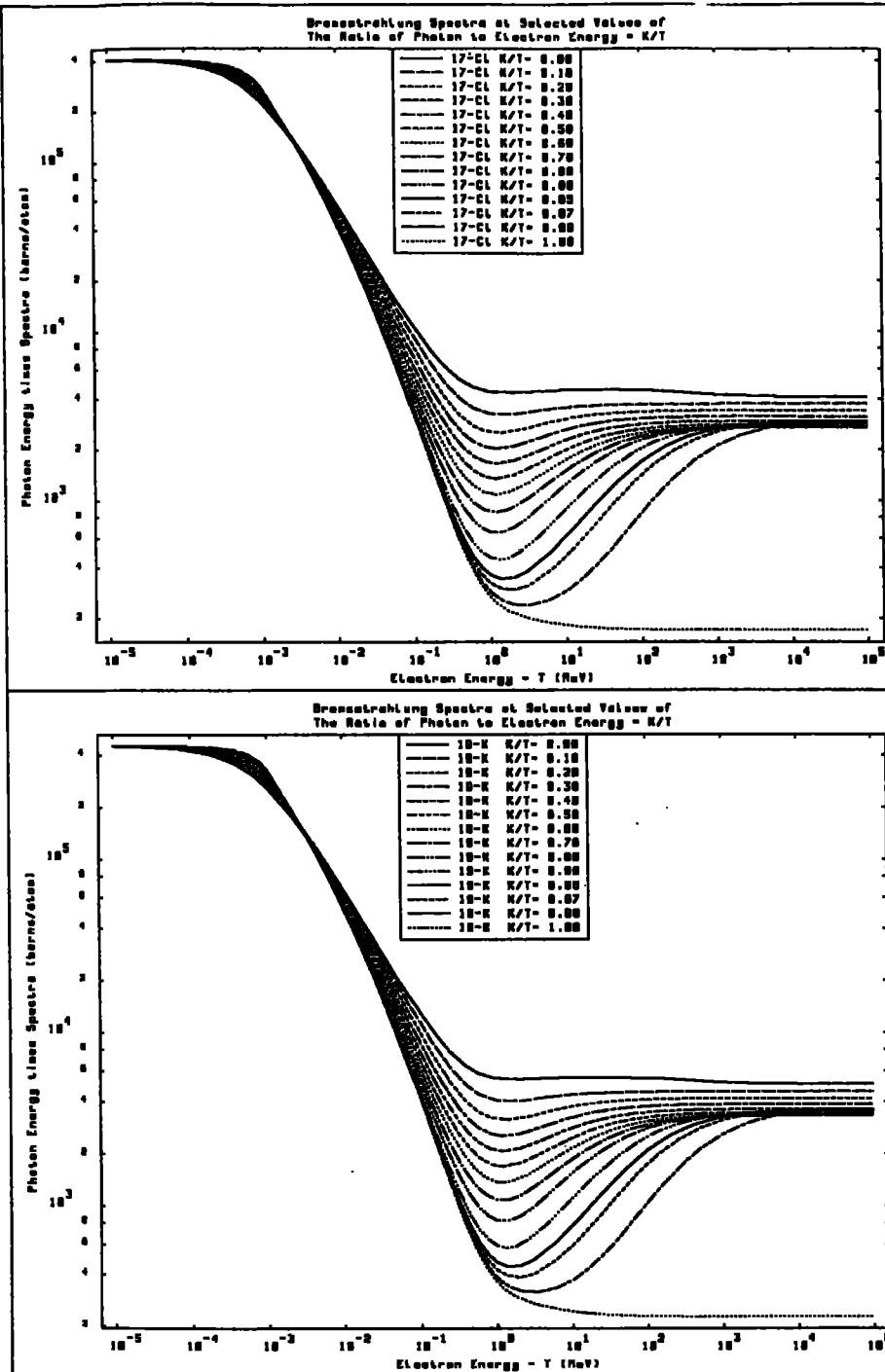
Note, the presentation in this form is similar to the form in which Seltzer and Berger presented their results (see Refs. 1 and 2), except that here the data has been extended to the energy range 10 eV to 100 GeV and also transformed from the variable used by Seltzer and Berger to the actual photon energy times the spectra.

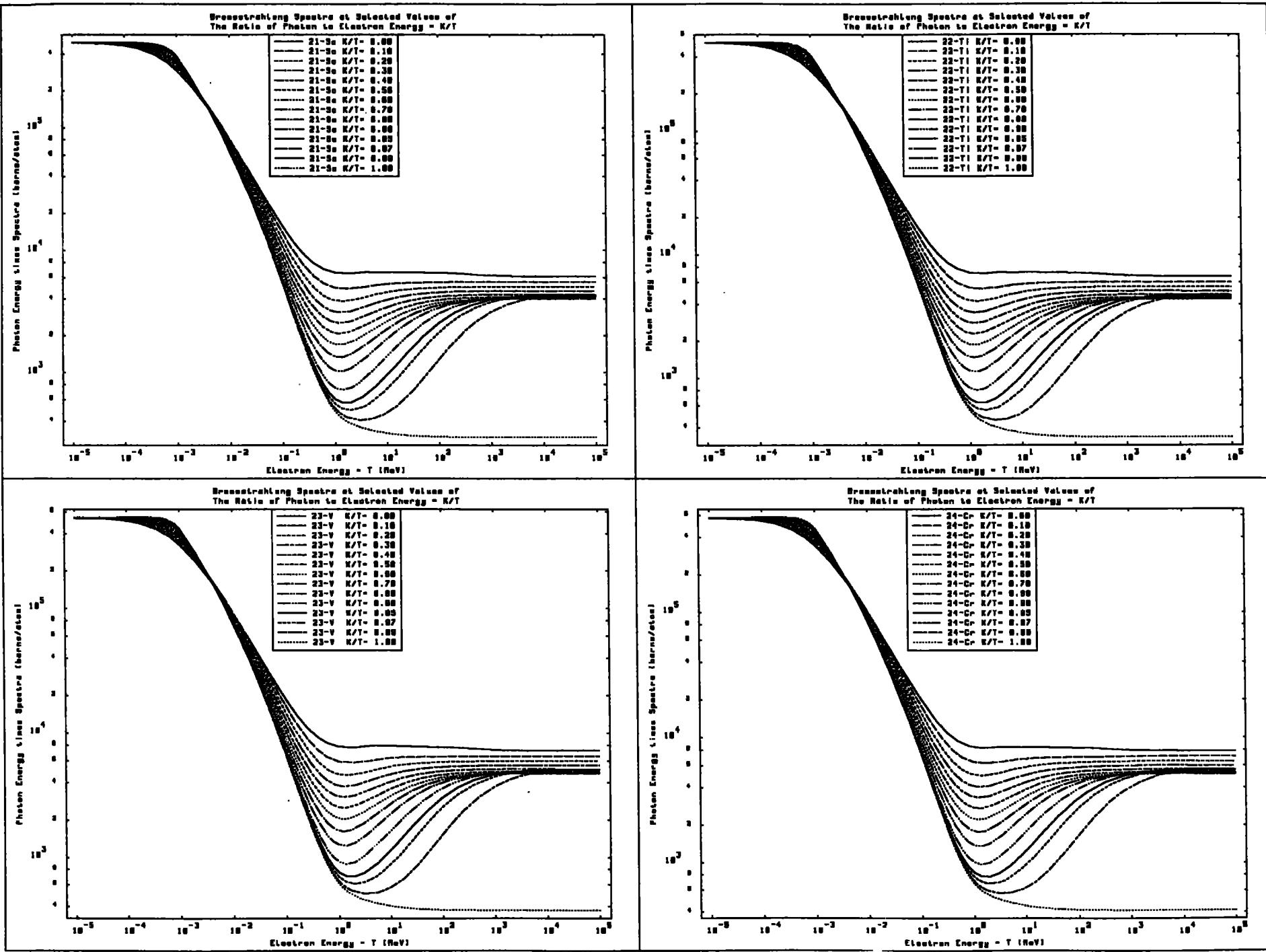


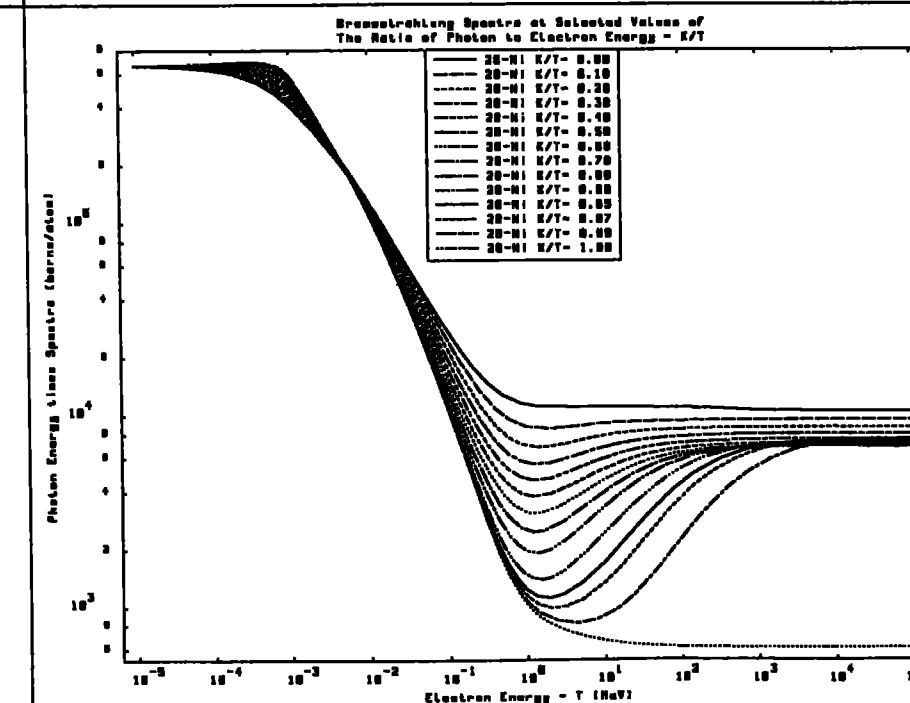
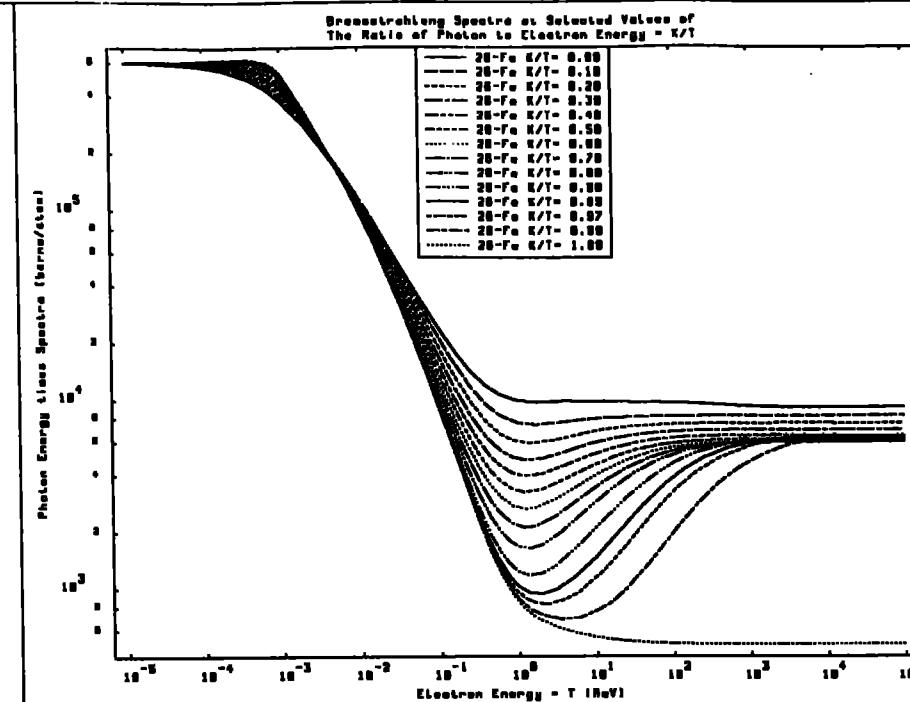
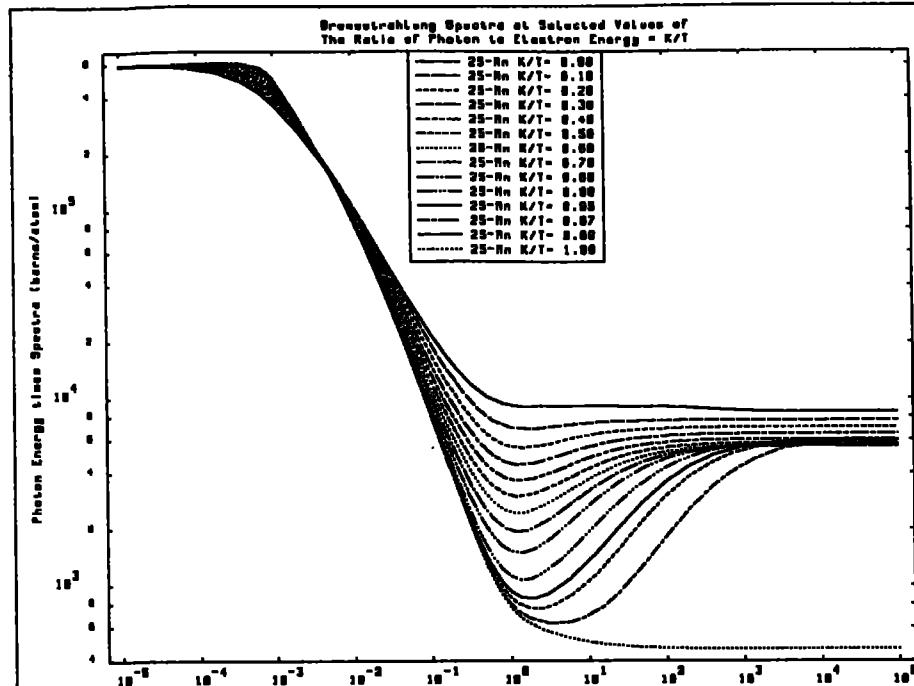




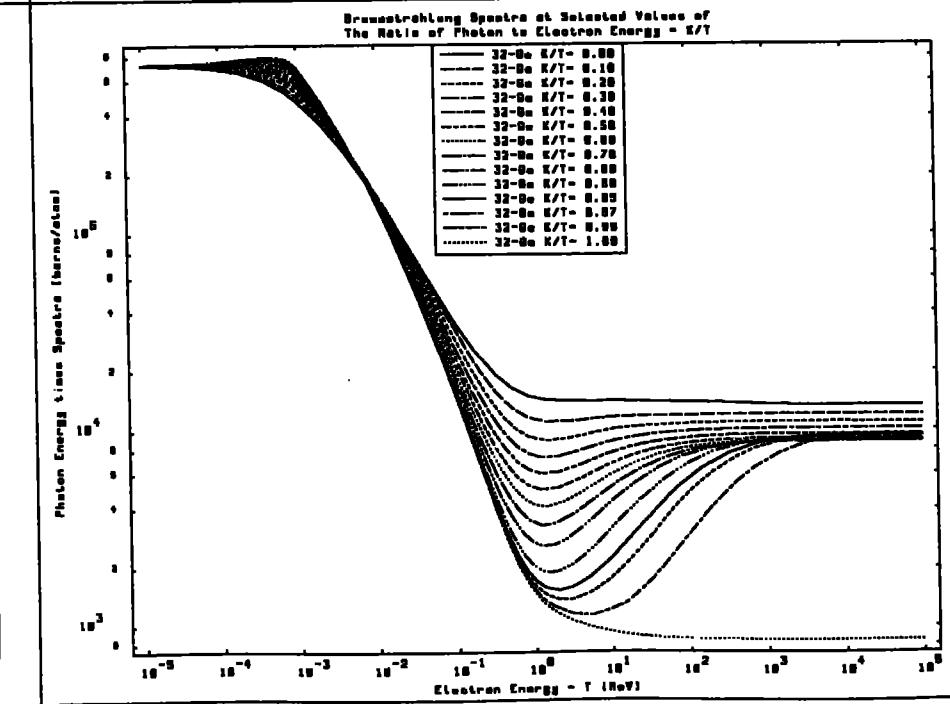
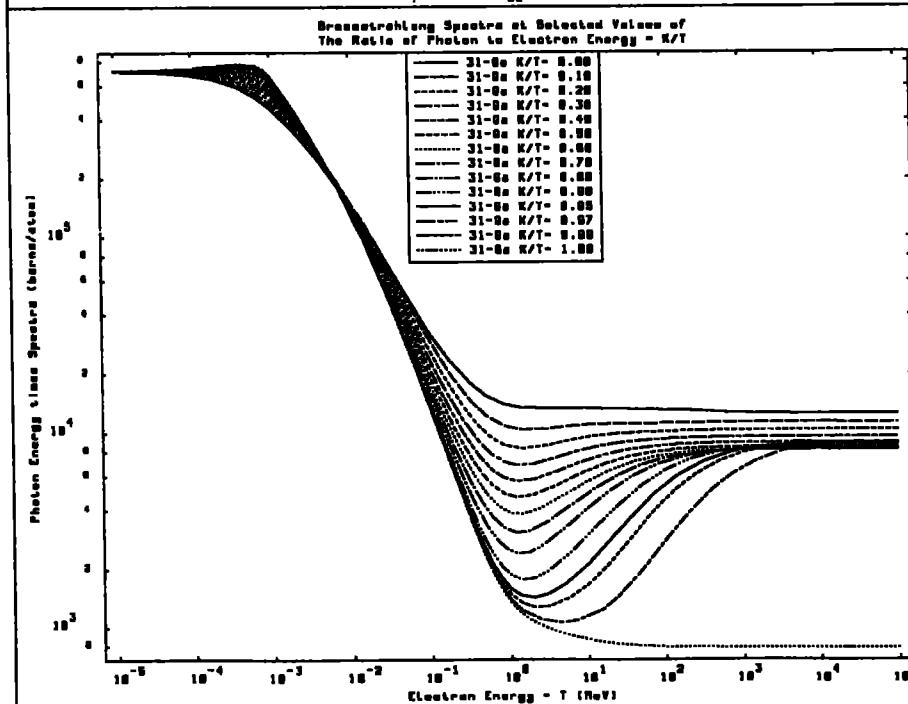
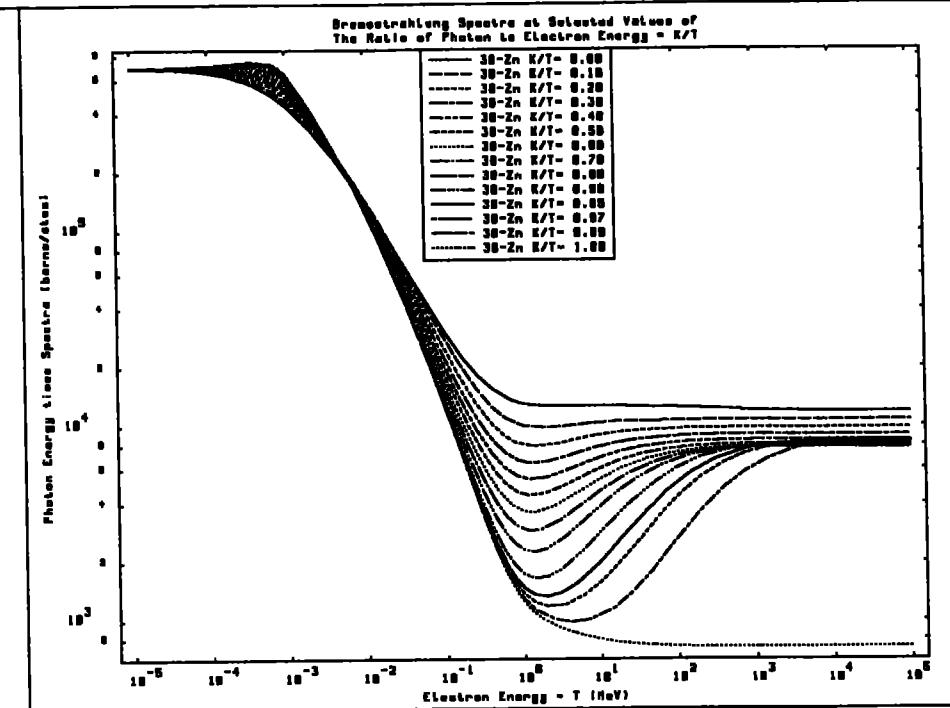
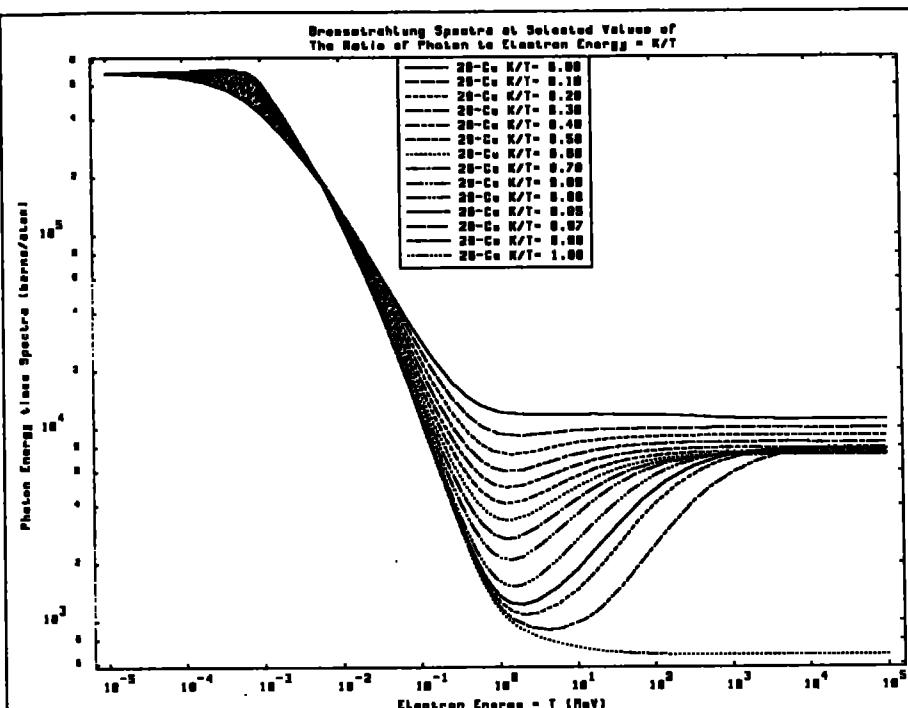




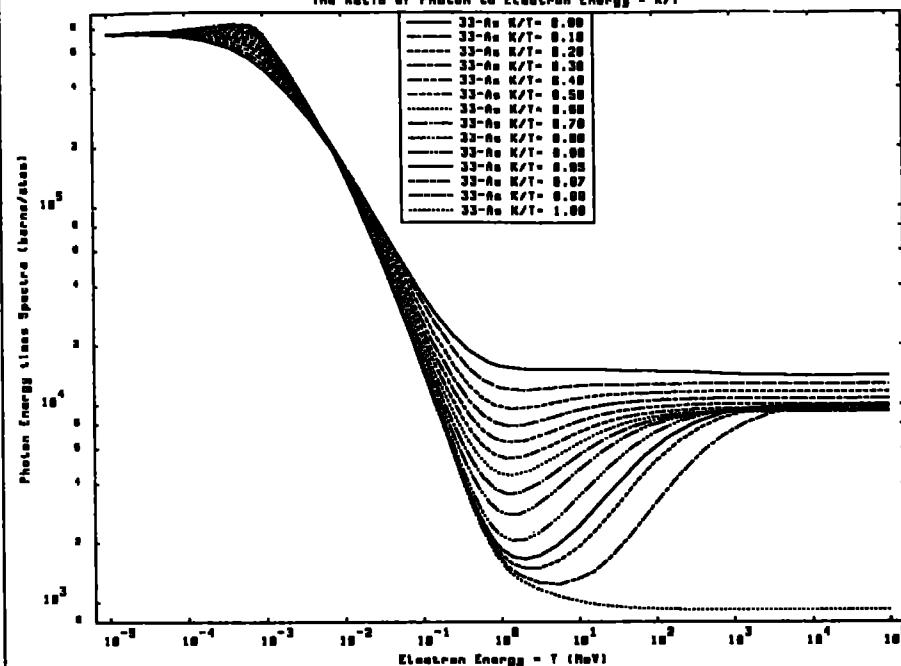




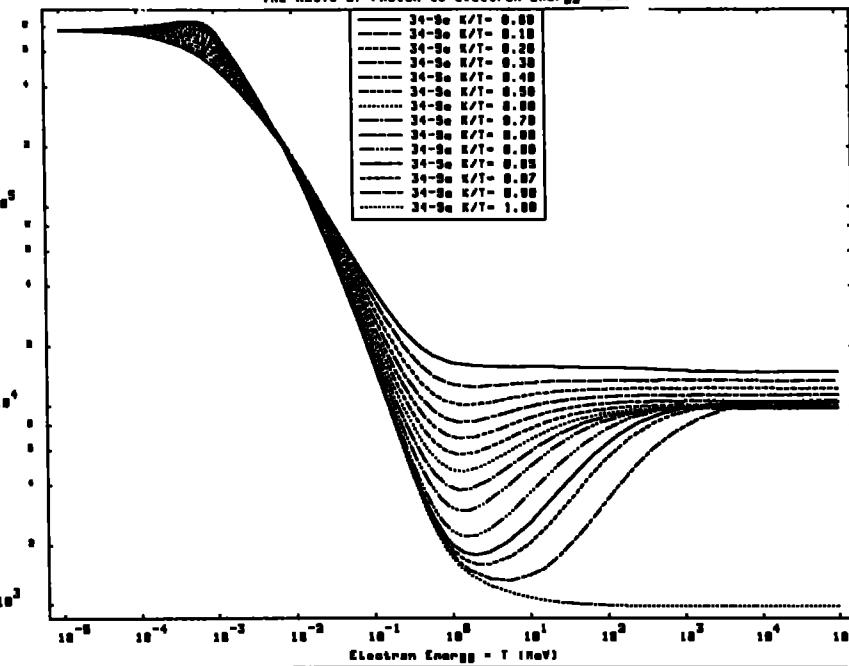
FILE: PLOTTABPLT DATE: Tue May 9 15:11:19 1989



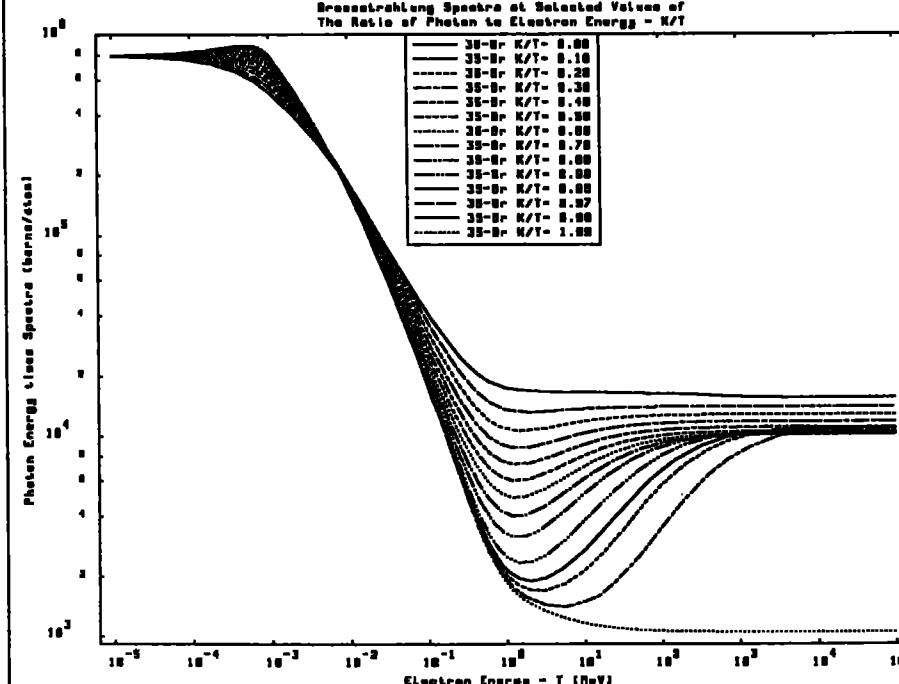
Bremsstrahlung Spectra at Selected Values of
The Ratio of Photon to Electron Energy = K/T



Bremsstrahlung Spectra at Selected Values of
The Ratio of Photon to Electron Energy = K/T



Bremsstrahlung Spectra at Selected Values of
The Ratio of Photon to Electron Energy = K/T



Bremsstrahlung Spectra at Selected Values of
The Ratio of Photon to Electron Energy = K/T

